# Band theory in the context of the Hamilton-Jacobi formulation

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February 1, 2008

**Abstract**

In the one-dimensional periodic potential case, we formulate the condition of Bloch periodicity for the reduced action by using the relation between the wave function and the reduced action established in the context of the equivalence postulate of quantum mechanics. Then, without appealing to the wave function properties, we reproduce the well-known dispersion relations which predict the band structure for the energy spectrum in the Krönig-Penney model.

PACS: 03.65.Ca; 03.65.Ta; 71.20.-b
Key words: quantum Hamilton-Jacobi equation, reduced action, Bloch theorem, band structure.

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# 1 Introduction

By establishing that quantum mechanics can be reproduced from an equivalence postulate [1, 2, 3], Faraggi and Matone have rekindled the hope that general relativity can be reconciled with quantum mechanics. Assuming that all quantum systems can be connected by a coordinate transformation, they derived the one-dimensional quantum stationary Hamilton-Jacobi equation

$$\frac{1}{2m}\left(\frac{\partial S_0}{\partial x}\right)^2 + V(x) - E = \frac{\hbar^2}{4m}\left[\frac{3}{2}\left(\frac{\partial S_0}{\partial x}\right)^{-2}\left(\frac{\partial^2 S_0}{\partial x^2}\right)^2 - \left(\frac{\partial S_0}{\partial x}\right)^{-1}\frac{\partial^3 S_0}{\partial x^3}\right] , \tag{1}$$

in which $V(x)$ is an external potential and $E$ the energy. They established then that the Schrödinger wave function is related to the reduced action, $S_0$, by

$$\phi(x) = R(x)\left[\alpha\ \exp\left(\frac{i}{\hbar}S_0(x)\right) + \beta\ \exp\left(-\frac{i}{\hbar}S_0(x)\right)\right] , \tag{2}$$

as shown also in [4] by using the probability current. In Eq. (2), $\alpha$ and $\beta$ are complex constants, $S_0(x)$ and $R(x)$ are real functions and $R(x)$ is proportional to $(\partial S_0/\partial x)^{-1/2}$. In contrast to Bohm's theory [5, 6], relation (2) guarantees that $S_0$ is never constant even in the case where the wave function is real, up to a constant phase factor. We note that the Bohm ansatz is obtained from (2) by using the particular values $\alpha = 1$ and $\beta = 0$.

Furthermore, without appealing to the usual axiomatic interpretation of the wave function, Faraggi and Matone [3, 7] showed that tunnel effect and energy quantization are consequences of the equivalence postulate. In the same spirit, we propose in this paper to examine the case of a system in a periodic potential. In section 2, we establish the condition of Bloch periodicity [8] for the reduced action. In section 3, we investigate the Krönig-Penney model [9] without appealing to the Schrödinger wave function or to its usual axiomatic interpretation. Section 4 is devoted to conclusion.

# 2 The Bloch theorem

The understanding of the behavior of electrons in crystal lattices has been advanced through the work of Bloch [8]. The main idea is that the interaction of an electron with the other particles of the lattice may be replaced by a periodic potential.

In the present work, we consider the one-dimensional case with a potential satisfying the following periodicity condition

$$V(x+e) = V(x), \qquad \forall\ x\ , \tag{3}$$

where $e$ is a period. With this relation, Bloch [8] showed that any solution $\phi$ of the Schrödinger equation,

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V(x)\phi = E\phi\ , \tag{4}$$

satisfies the property

$$\phi(x+e) = \exp(iKe)\,\phi(x) \;, \tag{5}$$

where $K$ is a constant. This property represents the condition of Bloch periodicity for the wave function. It is known as a Bloch theorem and was also established by Floquet [10].

Our task now consists in finding a corresponding version when we deal with the reduced action which is related to the wave function by (2). For this purpose, let us set

$$\alpha = |\alpha| \;\exp(ia) \;, \qquad\qquad \beta = |\beta| \;\exp(ib) \;, \tag{6}$$

$a$ and $b$ being real parameters. By substituting expressions (6) in (2), we can deduce that

$$\begin{aligned}
\exp(iKe)\;\phi(x) = \exp\left(i\frac{a+b}{2}\right) R(x) & \\
\Bigg\{ \Bigg[ (|\alpha|+|\beta|)\;\cos\left(\frac{S_0(x)}{\hbar}+\frac{a-b}{2}\right)\cos Ke & \\
-(|\alpha|-|\beta|)\;\sin\left(\frac{S_0(x)}{\hbar}+\frac{a-b}{2}\right)\sin Ke \Bigg] & \\
+i\Bigg[ (|\alpha|-|\beta|)\;\sin\left(\frac{S_0(x)}{\hbar}+\frac{a-b}{2}\right)\cos Ke & \\
+(|\alpha|+|\beta|)\cos\left(\frac{S_0(x)}{\hbar}+\frac{a-b}{2}\right)\sin Ke \Bigg] \Bigg\} &
\end{aligned} \tag{7}$$

Writing an analogous relation for $\phi(x+e)$ as in (2) and using (6), we obtain

$$\begin{aligned}
\phi(x+e) = \exp\left(i\frac{a+b}{2}\right) R(x+e) & \\
\Bigg[ (|\alpha|+|\beta|)\;\cos\left(\frac{S_0(x+e)}{\hbar}+\frac{a-b}{2}\right) & \\
+\, i(|\alpha|-|\beta|)\;\sin\left(\frac{S_0(x+e)}{\hbar}+\frac{a-b}{2}\right)\Bigg] &
\end{aligned} \tag{8}$$

Substituting (7) and (8) in (5) and separating in the obtained relation the real part from the imaginary one, we get to the two following relations

$$\begin{aligned}
(|\alpha|+|\beta|)\,R\,(x+e)\cos\left(\frac{S_0\,(x+e)}{\hbar}+\frac{a-b}{2}\right) = & \\
R\,(x)\left[(|\alpha|+|\beta|)\cos\left(\frac{S_0\,(x)}{\hbar}+\frac{a-b}{2}\right)\cos Ke\right. & \\
\left. -\,(|\alpha|-|\beta|)\sin\left(\frac{S_0\,(x)}{\hbar}+\frac{a-b}{2}\right)\sin Ke\right] &
\end{aligned} \tag{9}$$

and

$$\begin{aligned}
(|\alpha|-|\beta|)\,R\,(x+e)\sin\left(\frac{S_0\,(x+e)}{\hbar}+\frac{a-b}{2}\right) = & \\
R\,(x)\left[(|\alpha|-|\beta|)\sin\left(\frac{S_0\,(x)}{\hbar}+\frac{a-b}{2}\right)\cos Ke\right. & \\
\left. +\,(|\alpha|+|\beta|)\cos\left(\frac{S_0\,(x)}{\hbar}+\frac{a-b}{2}\right)\sin Ke\right] . &
\end{aligned} \tag{10}$$

Dividing side by side relations (10) and (9), we obtain

$$\Gamma \tan\left[\frac{S_0\,(x+e)}{\hbar}+\Delta\right]=\frac{\Gamma\tan\left[S_0\,(x)\,/\hbar+\Delta\right]+\tan Ke}{1-\Gamma\tan\left[S_0\,(x)\,/\hbar+\Delta\right]\tan Ke} \tag{11}$$

where

$$\Delta=\frac{a-b}{2}\ , \qquad\qquad \Gamma=\frac{|\alpha|-|\beta|}{|\alpha|+|\beta|}\ . \tag{12}$$

Knowing that $\tan\,(\arctan u)=u\ \forall\ u\in\Re$, with the use of

$$u=\Gamma\tan\left[\frac{S_0(x)}{\hbar}+\Delta\right]\ ,$$

relation (11) turns out to be

$$\begin{aligned}\arctan\left\{\Gamma\tan\left[\frac{S_0\,(x+e)}{\hbar}+\Delta\right]\right\}=&\\ \arctan\left\{\Gamma\tan\left[\frac{S_0\,(x)}{\hbar}+\Delta\right]\right\}&+Ke+n\pi\end{aligned} \tag{13}$$

where $n$ is an integer number. This relation is the condition of Bloch periodicity for the reduced action and represents the Bloch theorem version in this context. Taking into account the relation $\tan\alpha=-i[\exp(2i\alpha)-1][\exp(2i\alpha)+1]^{-1}$, it is easy to show from (11) that the periodicity condition (13) can be written in the following form

$$\exp[2iS_0(x+e)/\hbar]=\frac{P\exp[2iS_0(x)/\hbar]+Q}{M\exp[2iS_0(x)/\hbar]+N}\ , \tag{14}$$

where

$$\begin{aligned}P&=-(1-\Gamma)^2+(1+\Gamma)^2\exp(2iKe)\ , &(15)\\ Q&=(1-\Gamma^2)[\exp(2iKe)-1]\exp(-2i\Delta)\ , &(16)\\ M&=-(1-\Gamma^2)[\exp(2iKe)-1]\exp(2i\Delta)\ , &(17)\\ N&=(1+\Gamma)^2-(1-\Gamma)^2\exp(2iKe)\ . &(18)\end{aligned}$$

Relation (14) indicates that $\exp[2iS_0(x+e)/\hbar]$ is the Möbius transformation of $\exp[2iS_0(x)/\hbar]$. The Möbius group has allowed to fix from the equivalence postulate the quantum version of the Hamilton-Jacobi equation [3]. The trace of the Möbius transformation (14) is $P+N=4\Gamma[1+\exp(2iKe)]$. Except for the particular values of $K$ with which $\sin Ke$ vanishes, this trace is complex and hence the transformation (14) can not be classified as hyperbolic, parabolic or elliptic [11]. In the case of Bohm's theory, we have the particular values $\alpha=1$ and $\beta=0$ which imply that $\Gamma=1$ and $\Delta=0$. It follows that both relations (13) and (14) reduce to

$$S_0\,(x+e)=S_0\,(x)+\hbar Ke+n'\pi\hbar\ , \tag{19}$$

where $n'$ is also an integer number. It is interesting to observe that if we define the function

$$F(x)\equiv\frac{1}{\pi\hbar}[S_o(x)-\hbar Kx]\ , \tag{20}$$

we can show from (19) the following affine transformation

$$F(x+e)=F(x)+n'\ . \tag{21}$$

## 3 The Krönig-Penney model

Another important step in the description of the behavior of electrons in crystal lattices was the work of Krönig and Penney [9]. In one dimension, their model, which has the advantage in that it predicts correctly the spectrum of permissible energy values, consists in considering the potential in the form of a series of equidistant rectangular barriers

$$V(x) = \begin{cases} 0, & n(c+d) < x < n(c+d) + c \\ V_0, & n(c+d) + c < x < (n+1)(c+d) \end{cases} ,$$

where $n$ is an integer number. The period is $e = c + d$.

Let us begin by the case where $E > V_0$ and set

$$k_1 = \frac{\sqrt{2m(E - V_0)}}{\hbar} , \qquad k_2 = \frac{\sqrt{2mE}}{\hbar} . \tag{22}$$

In Refs. [12, 13], by using the continuity of the wave function and its derivative, it is shown that

$$\cos Ke = \cos(k_1 d) \cos(k_2 c) - \frac{k_1^2 + k_2^2}{2k_1 k_2} \sin(k_1 d) \sin(k_2 c) \tag{23}$$

An investigation of this dispersion relation shows the existence of a band structure for the energy spectrum.

Our goal now is to reproduce relation (23) by using the properties of the reduced action.

Let us call $I$, $II$ and $III$ the three regions $-d < x < 0$, $0 < x < c$ and $c < x < c + d$ respectively and impose the continuity at $x = 0$ for the reduced action and its first and second derivative

$$S_0^I(x)\big|_0 = S_0^{II}(x)\big|_0 , \tag{24}$$

$$\left.\frac{\partial S_0^I(x)}{\partial x}\right|_0 = \left.\frac{\partial S_0^{II}(x)}{\partial x}\right|_0 , \tag{25}$$

$$\left.\frac{\partial^2 S_0^I(x)}{\partial x^2}\right|_0 = \left.\frac{\partial^2 S_0^{II}(x)}{\partial x^2}\right|_0 . \tag{26}$$

Since $c = e - d$, by assuming at $x = -d$ the following continuity condition:

$$S_0^{III}(x+e)\big|_{x=-d} = S_0^{II}(x+e)\big|_{x=-d} ,$$

and by applying at $x = -d$ the condition of Bloch periodicity, Eq. (13), for the reduced action, we deduce that

$$\begin{aligned} &\arctan\left\{\Gamma \tan\left[\frac{S_0^{II}(x+e)}{\hbar} + \Delta\right]\right\}\Bigg|_{x=-d} = \\ &\qquad \arctan\left\{\Gamma \tan\left[\frac{S_0^{I}(x)}{\hbar} + \Delta\right]\right\}\Bigg|_{x=-d} + Ke + n\pi . \end{aligned} \tag{27}$$

As at $x = 0$, by assuming also the continuity at $x = -d$ of the first and the second derivative of $S_0(x+e)$,

$$\left.\frac{\partial S_0^{III}(x+e)}{\partial x}\right|_{x=-d} = \left.\frac{\partial S_0^{II}(x+e)}{\partial x}\right|_{x=-d} ,$$

$$\left.\frac{\partial^2 S_0^{III}(x+e)}{\partial x^2}\right|_{x=-d} = \left.\frac{\partial^2 S_0^{II}(x+e)}{\partial x^2}\right|_{x=-d} ,$$

we can take the first and the second derivative of the two sides of relation (27)

$$\left.\frac{\partial}{\partial x}\arctan\left\{\Gamma\tan\left[\frac{S_0^{II}(x+e)}{\hbar}+\Delta\right]\right\}\right|_{x=-d} = \left.\frac{\partial}{\partial x}\arctan\left\{\Gamma\tan\left[\frac{S_0^{I}(x)}{\hbar}+\Delta\right]\right\}\right|_{x=-d} , \tag{28}$$

$$\left.\frac{\partial^2}{\partial x^2}\arctan\left\{\Gamma\tan\left[\frac{S_0^{II}(x+e)}{\hbar}+\Delta\right]\right\}\right|_{x=-d} = \left.\frac{\partial^2}{\partial x^2}\arctan\left\{\Gamma\tan\left[\frac{S_0^{I}(x)}{\hbar}+\Delta\right]\right\}\right|_{x=-d} . \tag{29}$$

The solution for the one-dimensional quantum stationary Hamilton-Jacobi equation, Eq. (1), is well-known [1, 3, 4, 14, 15, 16] and is written in [17] as

$$S_0 = \hbar\ \arctan\left[\mu\frac{\phi_1}{\phi_2}+\nu\right]+\hbar l , \tag{30}$$

where $(\phi_1, \phi_2)$ is a couple of two real independent solutions of the Schrödinger equation, Eq. (4), and $(\mu, \nu, l)$ are real integration constants satisfying the condition $\mu \neq 0$. Let us choose for Eq. (4) the couples of independent solutions

$$(\sin k_1 x, \cos k_1 x), \qquad\qquad (\sin k_2 x, \cos k_2 x) \tag{31}$$

respectively in regions $I$ and $II$. With the use of (30), we have

$$S_0^I(x) = \hbar\ \arctan\left[\mu_1\tan(k_1 x)+\nu_1\right]+\hbar l_1 , \tag{32}$$

and

$$S_0^{II}(x) = \hbar\ \arctan\left[\mu_2\tan(k_2 x)+\nu_2\right]+\hbar l_2 . \tag{33}$$

As the reduced action is defined up to an additive constant, we can fix one constant among $(l_1, l_2)$ and determine the other from the boundary conditions. Thus, let us choose

$$l_1 = -\Delta , \tag{34}$$

where $\Delta$ is defined in (12), and apply relations (24), (25) and (26)

$$\hbar\ \arctan(\nu_1) - \hbar\Delta = \hbar\ \arctan(\nu_2)+\hbar l_2 , \tag{35}$$

$$\hbar\frac{\mu_1 k_1}{1+\nu_1^2} = \hbar\frac{\mu_2 k_2}{1+\nu_2^2} , \tag{36}$$

$$-\hbar\frac{2\mu_1^2\nu_1 k_1^2}{(1+\nu_1^2)^2} = -\hbar\frac{2\mu_2^2\nu_2 k_2^2}{(1+\nu_2^2)^2} \ . \tag{37}$$

From the system (35), (36) and (37), it is easy to show that

$$\begin{aligned} \nu_1 &= \nu_2 \ , & (38)\\ l_1 &= l_2 = -\Delta \ , & (39)\\ \mu_1 &= \frac{k_2}{k_1}\mu_2 \ , & (40) \end{aligned}$$

and relations (32) and (33) become

$$S_0^I(x) = \hbar \ \arctan\left[\mu_1\tan(k_1 x)+\nu_1\right] - \hbar\Delta \ , \tag{41}$$

and

$$S_0^{II}(x) = \hbar \ \arctan\left[\frac{k_1}{k_2}\mu_1\tan(k_2 x)+\nu_1\right] - \hbar\Delta \ . \tag{42}$$

As $c = e - d$, if we set

$$\begin{aligned} A &= -\mu_1\tan(k_1 d)+\nu_1 & (43)\\ B &= \frac{k_1}{k_2}\mu_1\tan(k_2 c)+\nu_1 & (44) \end{aligned}$$

relation (27) gives

$$\arctan\{\Gamma\tan[\arctan B]\} = \arctan\{\Gamma\tan[\arctan A]\} + Ke + n\pi \tag{45}$$

which leads to

$$\Gamma B = \frac{\Gamma A + \tan Ke}{1-\Gamma A\tan Ke} \ . \tag{46}$$

This relation can be rewritten in the following form

$$\cos^2 Ke = \frac{(1+\Gamma^2 AB)^2}{(1+\Gamma^2 A^2)(1+\Gamma^2 B^2)} \ . \tag{47}$$

With the use of (41), (42), (43) and (44), by applying successively (28) and (29), we find

$$(1+\Gamma^2 B^2)\cos^2 k_2 c = (1+\Gamma^2 A^2)\cos^2 k_1 d \tag{48}$$

and

$$\begin{aligned} &\frac{k_2\tan k_2 c}{(1+\Gamma^2 B^2)\cos^2 k_2 c} + \frac{k_1\tan k_1 d}{(1+\Gamma^2 A^2)\cos^2 k_1 d}\\ &\qquad = \frac{\mu_1 k_1\Gamma^2 B}{(1+\Gamma^2 B^2)^2\cos^4 k_2 c} - \frac{\mu_1 k_1 \Gamma^2 A}{(1+\Gamma^2 A^2)^2\cos^4 k_1 d} \ . \end{aligned} \tag{49}$$

Taking into account relations (48), (47) and (49) give respectively

$$\cos^2 Ke = \left(\frac{1+\Gamma^2 AB}{1+\Gamma^2 A^2}\right)^2 \frac{\cos^2 k_2 c}{\cos^2 k_1 d} \tag{50}$$

and

$$\Gamma^2(B-A) = \frac{1+\Gamma^2 A^2}{\mu_1 k_1}(k_2\tan k_2 c + k_1\tan k_1 d)\cos^2 k_1 d \ . \tag{51}$$

From (43) and (44), we write

$$B - A = \frac{\mu_1}{k_2}(k_1 \tan k_2 c + k_2 \tan k_1 d) \ . \tag{52}$$

Multiplying side by side relations (51) and (52) and using the identity

$$\Gamma^2 (B-A)^2 = (1+\Gamma^2 B^2) + (1+\Gamma^2 A^2) - 2(1+\Gamma^2 AB) \ , \tag{53}$$

we find

$$2(1+\Gamma^2 AB) = (1+\Gamma^2 A^2)\left[1 + \frac{1+\Gamma^2 B^2}{1+\Gamma^2 A^2} - \frac{W \cos^2 k_1 d}{k_1 k_2}\right] \ , \tag{54}$$

where

$$W = (k_1 \tan k_1 d + k_2 \tan k_2 c)(k_1 \tan k_2 c + k_2 \tan k_1 d) \ . \tag{55}$$

Using (48), (54) turns out to be

$$\frac{1+\Gamma^2 AB}{1+\Gamma^2 A^2} = \frac{1}{2}\left[1 + \frac{\cos^2 k_1 d}{\cos^2 k_2 c} - \frac{W \cos^2 k_1 d}{k_1 k_2}\right] \ , \tag{56}$$

Substituting this result in (50), we find

$$\cos Ke = \frac{1}{2}\left[1 + \frac{\cos^2 k_1 d}{\cos^2 k_2 c} - \frac{W \cos^2 k_1 d}{k_1 k_2}\right] \frac{\cos k_2 c}{\cos k_1 d} \tag{57}$$

Using expression (55) of $W$, this last relation leads straightforwardly to (23).

Let us now consider the case where $E < V_0$ and set

$$k_3 = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \ . \tag{58}$$

In Refs. [12, 13], by using the continuity of the wave function and its derivative, it is shown that

$$\cos Ke = \cosh(k_3 d)\cos(k_2 c) - \frac{k_2^2 - k_3^2}{2 k_2 k_3}\sinh(k_3 d)\sin(k_2 c) \tag{59}$$

This relation was obtained for the first time by Krönig and Penney [9]. As it is the case for (23), an investigation of (59) shows the existence of a band structure for the energy spectrum. In order to reproduce it with the use of the the reduced action properties, let us choose as independent real solutions of the Schrödinger equation, Eq. (4), the two couples

$$(\sinh k_3 x, \cosh k_3 x), \qquad\qquad (\sin k_2 x, \cos k_2 x) \tag{60}$$

respectively in regions $I$ and $II$. With the use of (30), we have

$$S_0^I(x) = \hbar \ \arctan\left[\mu_3 \tanh(k_3 x) + \nu_3\right] + \hbar l_3 \ , \tag{61}$$

and $S_0^{II}(x)$ keeps the same expression as in (33). By appealing to the continuity conditions (24), (25) and (26) at $x = 0$ for the reduced action and its derivatives, and to Bloch periodicity condition with its derivatives, Eqs. (27), (28) and (29),

and by following the same procedure as above, we get to relation (59) without using the wave function.

We would like to emphasize that, in order to reproduce the dispersion relations (23) and (59), the choice of the couples (31) and (60) of solutions of the Schrödinger equation used in the reduced action is not an essential. Since the Schrödinger equation is linear, other choices which must be linear combinations of the above solutions are also possible. However, any other choice must reproduce the same dispersion relations. In fact, as shown in Ref. [18], we can check that the reduced action is invariant under any linear transformation of the solutions of the Schrödinger equation by redefining suitably the integration constants $(\mu, \nu, l)$.

# 4 Conclusion

The present work can be summarized in two main results.

1. In a periodic potential case, we established the condition of Bloch periodicity for the reduced action by using the relation between the wave function and the reduced action established in the context of the equivalence postulate of quantum mechanics. The analogous version of this theorem in Bohm's theory is also deduced.

2. In this context, by using the quantum Hamilton-Jacobi equation, we also reproduced the well-known dispersion relations which predict a band structure for the energy spectrum without appealing to the wave function or to its usual axiomatic interpretation. These relations can be also reproduced in the context of the Bohm theory which appears here as a particular case in which we take $(\alpha = 1, \beta = 0)$ and then $(\Gamma = 1, \Delta = 0)$.

To conclude, we think that the present work is a further argument to reinforce the belief that the equivalence postulate of quantum mechanics constitutes a serious alternative to the standard quantum mechanics. In fact, firstly it allows to reproduce the well-known results as it was already the case both for the tunnel effect and energy quantization [3, 7]. Secondly, it provides an appropriate frame to reconcile general relativity with quantum mechanic.

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